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Construction of a unique metric in quasi-Hermitian quantum mechanics: non-existence of the charge operator in a 2×2 matrix model

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Abstract

For a specific exactly solvable 2×2 matrix model with a $\mathcal{PT}$-symmetric Hamiltonian possessing a real spectrum, we construct *all* the eligible physical metrics $\Theta > 0$ and show that *none* of them admits a factorization $\Theta = \mathcal{CP}$ in terms of an involutive charge operator $\mathcal{C}$. Alternative ways of restricting the physical metric to a unique form are briefly discussed.

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1 Introduction

The recent perceivable growth of interest in quasi-Hermitian Hamiltonians $H \neq H^\dagger$ with real spectra (cf. the Appendix for a brief description) has, amongst other reasons, received an impetus from their possible deep relevance in field theory [1]. Using several numerical methods the authors of the latter pioneering letter demonstrated that the family of the manifestly non-Hermitian Hamiltonians

$$H = H(\nu) = -\frac{\hbar^2}{2m^2}\frac{d^2}{dx^2} + x^2(\mathrm{i}x)^\nu, \qquad \nu \geq 0 \tag{1}$$

possess (only) real energies $E_n(\nu)$ which smoothly vary with the exponent $\nu > 0$. In the limit $\nu \to 0^+$ this spectrum coincides with the well-known harmonic oscillator equidistant set $E_n(0) = 2n + 1$, $n = 0, 1, \ldots$ in units where $\hbar = 2m = 1$.

Although these observations have only been supported by rigorous proofs a few years later [2], the appealing contrast between the manifest *non*-Hermiticity of the Hamiltonian (1) and the strict absence of *any* instability of the levels ($\mathrm{Im}\, E_n = 0$ for all n) proved inspiring [3]. Bender and Boettcher's hypothesis that the manifest $\mathcal{PT}$-symmetry, $H(\nu)\mathcal{PT} = \mathcal{PT}\,H(\nu)$, of the Hamiltonian in question (where $\mathcal{P}$ indicates parity and $\mathcal{T}$ is complex conjugation [4]) underpins this property, has been confirmed by the strict reality of the spectrum in a number of exactly solvable examples [5]. Moreover, Mostafazadeh [6] then broadened the range of the hypothesis by pointing out that Hamiltonians with similar properties may be identified among all the pseudo-Hermitian operators which appear Hermitian in a suitable indefinite (pseudo)metric generalization η of parity,

$$H^\dagger = \eta\, H\, \eta^{-1}, \qquad \eta = \eta^\dagger\,. \tag{2}$$

Alternatively, in the light of the recent studies [7] one may select the "generalized parity" η in eq. (2) as a non-Hermitian operator, provided only that the product $\mathcal{S} = [\eta^{-1}]^\dagger\,\eta \neq I$ remains a symmetry of our Hamiltonian, $H\mathcal{S} = \mathcal{S}H$.

Coming full circle, the focus then returned to a re-discovery of the well-known fact that the compatibility of all similar models with the postulates of Quantum Mechanics necessitates that *besides* the property (2), *all* the models in question must *also* satisfy *another, independent* condition, termed quasi-Hermiticity [8]:

$$H^\dagger = \Theta\, H\, \Theta^{-1}, \qquad \Theta = \Theta^\dagger > 0\,. \tag{3}$$

The symbol Θ for the positive definite metric here replaces T, originally introduced in the paper [8] (where the terminology *quasi-Hermitian* was coined), and which may now be confusing in view of the central role of the time-reversal operator $\mathcal{T}$ in $\mathcal{PT}$-symmetric quantum mechanics. In related more recent literature one also finds some alternative symbols, e.g. η_+ [6], $\mathcal{CP}$ [9], U [10], $\mathcal{PQ}$ [11], all of them referring to the metric in the Hilbert space $\mathcal{H}$ of physical states.

2 Ambiguity of the metric

One has to note and emphasize that the specification of the operator Θ from the Hamiltonian does not determine the metric uniquely [8]. Indeed, once we fix H, the linear eq. (3) may lead to many different positive and Hermitian solutions Θ ([12], cf. Appendix). The existing approaches to determine a unique Θ from subsidiary conditions include

- a systematic introduction of further "external" observables to complete, with the Hamiltonian, an irreducible set of observables. Requiring the associated operators A_1, A_2, ... to be quasi-Hermitian with respect to the *same* metric Θ, then completely eliminates any remaining freedom in Θ [8];

- a requirement that the metric Θ be factorized using a "charge" operator $\mathcal{C}$: $\mathcal{C} \equiv \Theta\,\mathcal{P}^{-1}$ [13], or "quasi-parity" $\mathcal{Q} \equiv \mathcal{P}^{-1}\,\Theta$ [14]. Then, the key idea of the reduction of the freedom in Θ relies on the "natural" involution properties $\mathcal{C}^2 = I$ and $\mathcal{Q}^2 = I$, respectively;

- a separable representation of Θ which enables one to fix the free constants in each term separately [15];

- a transition to the partial-differential-equation re-arrangement of the quasi-Hermiticity condition (3) which reduces the ambiguity of Θ by the specification of the related boundary conditions [16].

Some of these alternatives are discussed here via an explicit analysis of a schematic model.

2.1 A 2×2 matrix example

Consider an harmonic oscillator basis in which parity is explicitly indicated, $\{\, |n, \pm\rangle \,\}$. (Here $n = 0, 1, \ldots$ with parity $+$ or $-$). Generically [17], Hamiltonians $H(\nu)$ of the complex symmetric type (1) will take the schematic infinite-dimensional real, but *non-symmetric*, form

$$H(\nu) = \begin{pmatrix} S & B \\ -B^T & L \end{pmatrix}, \tag{4}$$

when represented in a basis which uses normalized states of the form $|n, +\rangle$ and $i|n', -\rangle$, with S and L symmetric, and B not necessarily so. (A specific example is the well studied imaginary potential $V(x) = ix^3$ which has non-zero matrix elemenets only between basis states with different parity; these matrix elements are then real with our choice of basis.)

The usual hermiticity property of Hamiltonians is here replaced by a matrix version of the pseudo-Hermiticity of H with respect to the indefinite (pseudo)metric *matrix* P,

$$[H(\nu)]^\dagger = P\, H(\nu)\, P^{-1}, \qquad P = P^{-1} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} = P^\dagger. \tag{5}$$

A "better" basis might have been chosen such that both the matrices S and L become diagonal.

In order to clarify the essence of the model (4) let us contemplate a violation of the parity by such an *ad hoc* potential which leaves just a single matrix element in the matrix B of eq. (4) different from zero, $B_{IJ} \neq 0$. In such a situation (with diagonal S and L) the coupling is only introduced between the $I-$th even energy S_{II} and the $J-$th odd energy L_{JJ}. Hence, the solution of the full Schrödinger equation degenerates to the analysis of the two-dimensional matrix problem

$$H \begin{pmatrix} x \\ y \end{pmatrix} = E \begin{pmatrix} x \\ y \end{pmatrix}, \qquad H = \begin{pmatrix} S_{II} & B_{IJ} \\ -B_{IJ} & L_{JJ} \end{pmatrix}. \tag{6}$$

In contrast to our previous considerations, we have to deal here with only three real matrix elements.

We emphasise that the $\mathcal{PT}$-symmetric matrix Hamiltonian (6) could also have been written down without any reference to the Hamiltonian (1), the present link only serving as additional motivation.

2.2 The metric Θ

For the sake of simplicity we may drop the subscripts and shift the origin of the energy scale in eq. (6),

$$H = \begin{pmatrix} -D & B \\ -B & D \end{pmatrix}, \qquad \mathcal{P} = \mathcal{P}^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \mathcal{P}^{\dagger}. \tag{7}$$

Remember that our first requirement is that all the eigenvalues, viz, the doublet

$$E_{\pm} = \pm\sqrt{D^2 - B^2}$$

remain real, i.e.,

$$B = D\,\cos\alpha, \qquad E_{\pm} = \pm D\,\sin\alpha, \qquad \alpha \in (0, \pi)\,.$$

We have to exclude both the endpoints $\alpha = 0, \pi$ where one encounters the exceptional point (i.e., the geometric and algebraic multiplicities of $E = 0$ become different there). Also the point $\alpha = \pi/2$ is not interesting since our Hamiltonian becomes diagonal and Hermitian there. Finally, we may choose any overall factor D and assume that $\alpha \in (0, \pi/2)$ without any loss of insight mediated by the model. Equation (7) becomes replaced by its still fully representative one-parametric $D = 1$ version

$$H = \begin{pmatrix} -1 & \cos\alpha \\ -\cos\alpha & 1 \end{pmatrix}. \tag{8}$$

To this Hamiltonian we now have to assign a Hermitian metric operator containing four real parameters in general,

$$\Theta = \begin{pmatrix} a & b + ic \\ b - ic & d \end{pmatrix}.$$

This operator must satisfy eq. (3), $\Theta H = H^T \Theta$. Insertion of this general form of Θ shows that the quasi-hermiticity condition (3) implies two restrictions on the parameters of the metric:

$$2b = -(a + d)\cos\alpha; \quad c = 0 \,. \tag{9}$$

We must furthermore demand that $b \neq 0 \neq a + d = 2Z$, otherwise the metric could not be positive (or negative) definite as required. In this notation we may put $a = Z(1 + \xi)$ and $d = Z(1 - \xi)$ with any real ξ.

The scale factor Z is again arbitrary and may be set equal to one. In this way we arrive at the most general solution of our present $N = 2$ version of eq. (3),

$$\Theta = \left(\begin{array}{cc} 1+\xi & -\cos\alpha \\ -\cos\alpha & 1-\xi \end{array} \right) . \tag{10}$$

For such a two-dimensional matrix family both the eigenvalues are available in closed form,

$$\theta_\pm = 1 \pm \sqrt{\xi^2 + \cos^2\alpha} \,.$$

It is simple to conclude that *both* of them remain non-degenerate and positive if and only if

$$1 > \sqrt{\xi^2 + \cos^2\alpha} > 0 \,. \tag{11}$$

This means that we may set

$$\xi = \sin\alpha \sin\gamma, \quad \gamma \in [0, \pi/2) \tag{12}$$

with one independent free real parameter γ. This completes our construction of the general metric Θ.

3 Viable restrictions to fix the metric

Although all the so-called $\mathcal{PT}-$symmetric Hamiltonians $H \neq H^\dagger$ with real spectra can be treated as Hermitian with respect to many nontrivial *ad hoc* metrics $\Theta \neq I$, the choice of restrictions to obtain a unique "physical" metric Θ_{phys} remains largely unchartered. Several aspects of this open problem may be discussed via our highly schematic two-state model.

A real and symmetric Θ may also be generated directly from the bi-orthogonal set of eigenstates of H whenever a pseudo-Hermitian Hamltonian is diagonalizable in a suitable bi-orthogonal basis (see Ref. ([6], and also eq. (18) in the Appendix below).

3.1 Establishing an irreducible set of observables

As we already mentioned, there have been several proposals to reduce the freedom in the choice of Θ which may be chosen as *any* solution of the operator eq. (3). In particular, the authors of Ref. [8] showed that one has *to choose* a set of irreducible or "natural" observables $\mathcal{A}_j$ *and to demand* that

$$[\mathcal{A}_j]^\dagger = \Theta\,\mathcal{A}_j\,\Theta^{-1} \tag{13}$$

for *all* of them. However, different choices will lead to different quantum mechanical frameworks, and there is no general algorithm whereby the set may be completed after an initial choice of an observable (or observables) has been made to supplement the Hamiltonian. Under such a scenario let us assume that the "natural" observables $\mathcal{A}_j$ will mimic the "irreducible" set of coordinates x and momenta p (as mentioned in ref. [8]) by being represented by the *Hermitian* matrices,

$$\mathcal{A}_j = \left(\begin{array}{cc} A_j & B_j \\ B_j & D_j \end{array} \right) .$$

Such a family of the observables, characterized, *a priori*, by the three real parameters A, B and D must remain compatible with the original quasi-Hermiticity constraint (13). This represents (for all possible j) the constraint

$$2\xi B = (D - A)\cos\alpha.$$

As the choice of $B = 0$ would imply that $\mathcal{A} \sim I$ are trivial, we are allowed to assume that $B \neq 0$. In this way the choice of a single $\mathcal{A}_1 = \mathcal{A}$ fixes the freedom in our physical metric operator completely,

$$\xi_{\text{phys}} = \frac{D - A}{2B}\cos\alpha\ .$$

We may conclude that the approach proposed in ref. [8] fixed the parameter in our toy metric and leads to unique "physics".

It is instructive to notice that for the latter purpose one, and only one, *general* auxiliary observable $\mathcal{A}_1$ proved sufficient in our schematic model. It will be interesting to find some other and, hopefully, less schematic models with this property, which seems to be reminiscent of one-dimensional standard quantum mechanics where x and p form an irreducible set, the Hamiltonian generally being an auxiliary or derived operator, $H = H(x, p)$.

3.2 Factorization in terms of a charge operator

Our final comment concerns the connection of our example with the popular postulate of the factorization $\Theta = \mathcal{CP}$ accompanied by the requirement that the factor $\mathcal{C}$ may be interpreted as an operator of a "charge" with the property $\mathcal{C}^2 = I$ (cf., e.g., ref. [9]. In our example we may easily derive the explicit formula

$$\mathcal{C}^2 = \begin{pmatrix} (1+\xi)^2 - \cos^2\alpha & 2\xi\cos\alpha \\ -2\xi\cos\alpha & (1-\xi)^2 - \cos^2\alpha \end{pmatrix}.$$

Obviously, the requirement $\mathcal{C}^2 = I$ implies that $\xi = 0$. This forces us to set $\cos\alpha = 0$. We see that this in fact eliminates *all* the nontrivial Hamiltonians in our family. In other words, for all the non-diagonal non-Hermitian models with $\alpha \neq \pi/2$ the *involutive* charge operator does not exist at all.

4 Conclusion

We have motivated and studied a particular 2×2 $\mathcal{PT}$-symmetric matrix Hamiltonian, characterizing and constructing from various points of view a *unique* positive definite metric which would render the Hamiltonian quasi-Hermitian, and thus amenable to a standard quantum mechanical interpretation.

We conclude that while it is possible to find such metrics, the insistence on factorisation, $\Theta = \mathcal{CP}$, which is usually enforced in $\mathcal{PT}$-symmetric quantum mechanics, is inapplicable here. Note in this respect that the Hamiltonian matrix (4) is non-symmetric, in contrast to the 2×2 model studied by Bender *et al* [13] for which a $\mathcal{C}$-operator had in fact been constructed. In general further work is called for to elucidate the construction and implications of various approaches to identify and implement a unique metric in quasi-Hermitian quantum mechanics.

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References

[1] C. M. Bender and S. Boettcher, Phys. Rev. Lett. 80 (1998) 4243.

[2] P. Dorey, C. Dunning and R. Tateo, J. Phys. A: Math. Gen. 34 (2001) 5679;

K. C. Shin, Commun. Math. Phys. 229 (2002) 543.

[3] F. M. Fernández, R. Guardiola, J. Ros and M. Znojil, J. Phys. A: Math. Gen. 31 (1998) 10105;

B. Bagchi, S. Mallik and C. Quesne, Mod. Phys. Lett. A 17 (2002) 1651;

A. Mostafazadeh, Class. Quantum Grav. 20 (2003) 155;

H. Langer and Ch. Tretter, Czech. J. Phys. 54 (2004) 1113;

Czech. J. Phys. 55 (2005) 1045 - 1192; issue dedicated to *Pseudo-Hermitian Hamiltonians in Quantum Mechanics.*

[4] C. M. Bender, S. Boettcher and P. N. Meisinger, J. Math. Phys. 40 (1999) 2201.

[5] A. Andrianov, F. Cannata, J.-P. Dedonder and M. V. Ioffe, Int. J. Mod. Phys. A 14 (1999) 2675;

M. Znojil, Phys. Lett. A 259 (1999) 220;

G. Lévai and M. Znojil, J. Phys. A: Math. Gen. 33(2000) 7165;

B. Bagchi and C. Quesne, Phys. Lett. A 273 (2000) 285;

M. Znojil, Phys. Lett. A. 285 (2001) 7;

M. Znojil and M. Tater, J. Phys. A: Math. Gen. 34 (2001) 1793;

S. Albeverio, S.-M. Fei and P. Kurasov, Lett. Math. Phys. 59 (2002) 227;

V. Jakubský, Czech. J. Phys. 54 (2004) 67;

A. Sinha and P. Roy, Czech. J. Phys. 54 (2004) 129;

H. Bíla, V. Jakubský, M. Znojil, B. Bagchi, S. Mallik and C. Quesne, Czech. J. Phys. 55 (2005) 1075.

[6] A. Mostafazadeh, J. Math. Phys. 43 (2002) 205 and 2814.

[7] M. Znojil, J. Phys. A: Math. Gen. 39 (2006) 4047;

M. Znojil, Phys. Lett. A (2006), to appear (quant-ph/0601048).

[8] F. G. Scholtz, H. B. Geyer and F. J. W. Hahne, Ann. Phys. (NY) 213 (1992) 74.

[9] C. M. Bender, D. C. Brody and H. F. Jones, Phys. Rev. Lett. 89 (2002) 0270401;

[10] H. F. Jones, J. Phys. A: Math. Gen. 38 (2005) 1741.

[11] M. Znojil,

in "Symmetry Methods in Physics", Ed. C. Burdik, O. Navratil and S. Posta, JINR, Dubna, 2004 (CD ROM, also hep-th/0408081).

[12] A. Mostafazadeh, J. Phys. A: Math. Gen. 38 (2005) 6557; erratum, *ibid* 8185;

A. Mostafazadeh, quant-ph/0508195.

[13] C. M. Bender, D. C. Brody, H. F. Jones, Phys. Rev. Lett. 93 (2004) 251601;

C. M. Bender, D. C. Brody and H. F. Jones, Phys. Rev. D 70 (2004) 025001; Erratum-ibid. D 71 (2005) 049901;

C. M. Bender and H. F. Jones, Phys. Lett. A 328 (2004) 102;

C. M. Bender, S. F. Brandt, J-H. Chen and Q. Wang, Phys. Rev. D 71 (2005) 065010.

[14] M. Znojil, Rendiconti del Circ. Mat. di Palermo, Ser. II, Suppl. 72 (2004) 211 (math-ph/0104012);

M. Znojil, J. Phys. A: Math. Gen. 39 (2006) 441.

[15] A. Mostafazadeh and A. Batal, J. Phys. A: Math. Gen. 37 (2004) 11645.

[16] F. G. Scholtz and H. B. Geyer, Phys. Lett. B 634 (2006) 84.

[17] M. Znojil, math-ph/0106021;

M. Znojil, J. Nonlin. Mat. Phys. 9, Suppl. 2 (2002) 122.

Appendix: Metrics $\Theta \neq I$ in Hilbert space

According to the standard postulates of Quantum Mechanics, the states of a given system may be represented by elements $|\psi\rangle$ of a Hilbert space $\mathcal{H}$, endowed by a positive definite metric Θ. The statement about the metric is mostly omitted, as the standard metric $\Theta = I$ in $L^2(-\infty, \infty)$ is assumed. A system is then fully characterized by a set of its observable characteristics, e.g. by the energy E and by some other real, measurable quantities a_i, $i = 2, 3, \ldots, N^{(\mathrm{obs})}$, expected to lie in some respective subsets $\mathcal{D}_i$ of $I\!R$.

As pointed out in Ref. [8] the framework of Quantum Mechnics remains intact when a positive definite metric $\Theta \neq I$ is introduced. In such a context the quantum description of any system requires that its observables a_i are represented by the operators A_i in $\mathcal{H}$ which are Hermitian with respect to the "physical" metric Θ,

$$A_i^\dagger = \Theta\, A_i\, \Theta^{-1}. \tag{14}$$

Such operators, including H, have been termed "quasi-Hermitian" in Ref. [8].

The concept re-emerged in the framework of $\mathcal{PT}-$symmetric Quantum Mechanics [1] where $H \neq H^\dagger$, so that, typically, one must solve not only the "direct" Schrödinger bound-state problem, but also its Hermitian conjugate partner,

$$H\,|n\rangle = E_n\,|n\rangle, \qquad \langle\langle n|\, H = \langle\langle n|\, E_n\,. \tag{15}$$

Here we employed the matrix-algebra-inspired "left-action" convention and introduced a double bra symbol $\langle\langle n|$ for the conjugate eigenkets of $H^\dagger$.

Focussing on the Hamiltonian $H \neq H^\dagger$ only, the spectrum may be degenerate (and/or complex where no $\Theta > 0$ exists), while the related set of wave functions may also prove incomplete in general. All such degeneracies will be skipped and avoided in this short exposition. Thus, we may assume the biorthogonality ($\langle\langle n|m\rangle = 0$ iff $m \neq n$) and completeness of our bound states, as well as the existence of a metric $\Theta \neq I$ in the Hilbert space, rendering the Hamiltonian quasi-Hermitian,

$$H^\dagger = \Theta\, H\, \Theta^{-1}\,, \qquad \Theta = \Theta^\dagger > 0\,. \tag{16}$$

(See Ref. [8] for more details.) The insertion of the formal spectral expansion

$$H = \sum_{n=0}^{\infty} |n\rangle\, \frac{1}{\langle\langle n|n\rangle}\, \langle\langle n| \tag{17}$$

into eq. (16) indicates that

$$\Theta = \sum_{n,m} |n\rangle\rangle \, s_{n,m} \, \langle\langle m| \, . \tag{18}$$

Inserting the spectral form (17) and this ansatz into the defining eq. (16), leads to the conclusion that the array of coefficients must remain diagonal, $s_{n,m} = \delta_{n,m} \, s_m$,

$$\Theta = \sum_{m} |m\rangle\rangle \, s_m \, \langle\langle m| \, . \tag{19}$$

These coefficients must be real (due to the Hermiticity requirement $\Theta = \Theta^\dagger$) and positive (in order to guarantee the positive-definiteness of $\Theta > 0$). This presents an explicit construction of the metric Θ, the remaining freedom in s_m of course again reflecting the fact that quasi-Hermiticity of the Hamiltonian alone does not determine the metric uniquely.